

First principles modeling of fast electron physics

Y Peysson, D Mazon, J F Artaud, A Ekedahl, J Hillairet, A Jardin, K Kroll, J Bielecki, D Dworak, M Scholz, et al.

▶ To cite this version:

Y Peysson, D Mazon, J F Artaud, A Ekedahl, J Hillairet, et al.. First principles modeling of fast electron physics. ICFRD 2020 - International conference on diagnostics for fusion reactors, ICPC (International Center Piero Caldirola), Sep 2021, Varenne, Italy. cea-03467619

HAL Id: cea-03467619 https://cea.hal.science/cea-03467619

Submitted on 6 Dec 2021

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers. L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

DE LA RECHERCHE À L'INDUSTRIE



www.cea.fr

First principles modeling of fast electron physics

Y. Peysson^{1*}, D.Mazon¹, J. F. Artaud¹, A. Ekedahl¹, J.Hillairet¹, A. Jardin², K. Kroll², J. Bielecki², D. Dworak², M. Scholz², J. Decker³ and WEST Team⁺

¹CEA/IRFM, F-13108, Saint-Paul-lez-Durance, France ²Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland ³EPFL, Swiss Plasma Center, CH-1015 Lausanne, Switzerland

* yves.peysson@cea.fr + http://west.cea.fr/WESTteam



Outline



- First principles modeling
- LUKE : a versatile tool for modeling fast electron physics
- Towards large scale quantitative simulations with LUKE
- SLUKE : a new framework for automatic LUKE modeling
- Conclusion and prospects



$$\mathbf{J}(\mathbf{x},t) = |e| \sum_{s} Z_{s} \iiint d^{3} \mathbf{p} f_{s}(\mathbf{x},\mathbf{p},t) \mathbf{p}/\gamma_{s}$$

Plasma : a 6-D time-dependent problem with multiple scales !

Y. Peysson et al.





- Recovering microscopic informations from macroscopic measurements (inversion) is an ill-posed problem : an infinity of solutions may explain the observations !
- First principles modeling try to by-pass this difficulty by rebuilding experimental results (synthetic diagnostics) from a set of microscopic physical processes considering assumptions that reflect the multiple scales problem (time/space ordering)
- The uniqueness of the solution provided by first principles modeling is not guaranteed by this procedure. But extensive comparisons between calculations and observations may validate the description within a given parameters space → *large number of simulations*





- Microscopic scale : exact local physical processes in 6-D phase space
- Mesoscopic scale (kinetic) : time/space ordering (code modularity)
 - Curvilinear metrics
 - Dimension reduction 6-D \rightarrow 1-D (radial) + 2-D (momentum) Hamiltonian theory (Lie transform), symmetry or local averaging
- *Macroscopic scale (fluid)* : global averaging \rightarrow *diagnostics*
 - o Geometry
 - o Energy

Length ordering in a magnetized tokamak plasma





DE LA RECHERCHE À L'INDUSTRIE

Frequency ordering in a magnetized plasma









- Fast electrons play an important role in tokamak plasmas for steady-state operation, MHD stability, plasma heating,...
- Fast electrons can be driven :
 - by large inductive electric fields \rightarrow *runaways*
 - by resonant interactions with RF waves → heating & CD
- Their dynamics depends of the toroidal MHD equilibrium but also may impact it → self-consistency
- Fast electrons dynamics may be also perturbed by plasma fluctuations and MHD activity

General scheme for first principle modeling of fast electron physics with RF waves



Main modeling tools for RF electron waves



R.W. Harvey and M.G. McCoy, IAEA Conf. Proc. (1992) 489

Y. Peysson et al., EPJ Web of Conferences, 157 (2017) 02007



LUKE kernel : code set-up





Weak damping approximation \rightarrow code modularity

Y. Peysson and J. Decker, Fusion Science and Technology, 65 (2014) 22

Y. Peysson, J. Decker, et al. PPCF, 53 (2011) 124028





- Curvilinear coordinate system: $(\rho(\psi), \theta, \phi)$
- 2-D axisymmetric configuration (cylinder, dipole, torus) + 3-D perturbation (nested magnetic flux surfaces)
- Vectorization of the magnetic equilibrium: Fourier series + piecewise cubic interpolation using Hermite polynomials: no interpolation performed at each time step
- (4,5) order Runge-Kutta
- Rays are calculated inside the separatrix. Specular reflexion enforced - if needed - at ρ=1.

 Rays calculations are almost stopped when the rf power is linearly damped

- Cold, warm, hot and relativistic dielectric tensors
- Non-resonant collisional absorption (for very cold plasmas)
- Written in C (MatLab mex-file)

Y. Peysson et al., PPCF 54 (2012) 045003





Separation between **plasma dispersion models** and the metric associated to the magnetic equilibrium

$$\frac{\partial \mathbb{X}_{ij}^{s}}{\partial \mathbf{Y}} = \frac{\partial \mathbb{X}_{ij}^{s}}{\partial n_{\perp}} \frac{\partial n_{\perp}}{\partial \mathbf{Y}} + \frac{\partial \mathbb{X}_{ij}^{s}}{\partial n_{\parallel}} \frac{\partial n_{\parallel}}{\partial \mathbf{Y}} + \frac{\partial \mathbb{X}_{ij}^{s}}{\partial \beta_{Ts}} \frac{\partial \beta_{Ts}}{\partial \mathbf{Y}} + \frac{\partial \mathbb{X}_{ij}^{s}}{\partial \overline{\omega}_{ps}} \frac{\partial \overline{\omega}_{ps}}{\partial \mathbf{Y}} + \frac{\partial \mathbb{X}_{ij}^{s}}{\partial \overline{\Omega}_{s}} \frac{\partial \overline{\Omega}_{s}}{\partial \mathbf{Y}} \mathbf{Y} = (\mathbf{X}, \mathbf{k}, t, \omega) \beta_{s} = \sqrt{kT_{s}/m_{s}c^{2}} \overline{\omega}_{ps} = \omega_{ps}/\omega \qquad \overline{\Omega}_{s} = \Omega_{s}/\omega$$

Y. Peysson et al., 2012 Plasma Phys. Control. Fusion 54 045003

Y. Peysson et al.





- Linearized relativistic collision operator with partial screening (for W)
- Kennel-Engelman-Lerche relativistic rf diffusion operator
- Runaway electron physics with avalanches and ALD effect
- Curvilinear coordinate system (ψ, θ, ϕ)
- 2-D axisymmetric configuration (cylinder, torus, dipole)
- 3-D perturbation (nested magnetic flux surfaces)
- Non-uniform grids (f and fluxes)
- Fully implicit or Crank-Nicholson time schemes
- Chang & Cooper interpolation for non-uniform p grid (f_M) and linear interpolation for radial and pitch-angle grids
- Discrete cross-derivatives consistent with boundary conditions (stable scheme for $D_{ql} >> 1$)
- Written in MatLab

 Generalized incomplete LU factorization technique for an arbitrary number of non-zero diagonals (highly sparse L and U matrices, low memory consumption).
 External iterative solvers MUMPS,...

Y. Peysson and J. Decker, Fusion Science and Technology, 65 (2014) 22

The 3-D linearized bounce-averaged relativistic Fokker-Planck solver LUKE



• Fully 3-D conservative formulation $\frac{\partial f^{(0)}}{\partial t} + \nabla \cdot \mathbf{S}^{(0)} = s_{+}^{(0)} - \underline{s_{-}^{(0)}}$ $\frac{\partial f^{(0)}}{\delta \psi} \left(\frac{\tilde{q}\lambda}{B_{0}} \| \nabla \psi \| S_{\psi}^{(0)} \right)$ momentum space

 $\overline{\lambda p} \,\overline{\partial \xi}_0$

configuration space

Orbit effect

Magnetic ripple losses

$$\mathbf{S}^{(0)} = -\mathbb{D}^{(0)} \cdot \nabla f^{(0)} + \mathbf{F}^{(0)} f^{(0)}$$

J. Decker, and Y. Peysson, report EUR-CEA-FC-1736, Euratom-CEA (2004)

Y. Peysson and J. Decker, Fusion Science and Technology, 65 (2014) 22



Reduced configuration space: 3-D





All the electron dynamics is projected at $B = B_{min}$

Thin banana width

Bounce-averaged electron momentum distribution function



Momentum space dynamics on the magnetic flux surface $\,\psi$

Y. Peysson et al.

DE LA RECHERCHE À L'INDUSTRIE

Fokker-Planck matrix to be inverted



Y. Peysson, et al., 15th Top. Conf. on Radio Frequency Power in Plasmas, 2003, vol. 694 of AIP Conf. Proc., pp. 495–498.

de la recherche à l'industrie

LHW absorption: rf diffusion in Fokker-Planck calculations. Link between C3PO and LUKE.





Ray fragment in layer at $\psi_{\text{I+1/2}},\!\theta_{\text{b}}$

J. Decker and Y. Peysson, EUR-CEA-FC-1736 report (2004)

Y. Peysson et al.

 RF power flows almost instantaneously from initial ray position to the last calculated point since

$$v_G/L_{ray} \ll au_{bounce} \ll au_{coll}$$

 Each ray is split in small fragments depending on the number of plasma layers.

 \mathcal{P}_i : RF power carried by the ray fragment i,

$$D_{\parallel}(\psi, p_{\parallel}, p_{\perp}) = \sum_{i} \frac{\mathcal{P}_{i}}{\mathcal{P}_{i0}} \frac{D_{\parallel i}}{\sqrt{\pi} \Delta n_{\parallel i}} \exp\left[-\frac{\left(n_{\parallel i} - n_{\parallel res}\right)^{2}}{\Delta n_{\parallel i}^{2}}\right]$$

 $n_{||\text{res}} = c/v_{||}$: resonance condition at position ($\psi_{l+1/2}, \theta_b$) $Q_{\text{LH}}(f) = \frac{\partial}{\partial p_{||}} D_{||} \frac{\partial f}{\partial p_{||}}$: RF diffusion operator

 $\frac{\partial f}{\partial t} = C(f) + Q_{\text{LH}}(f) + \cdots$: Fokker-Planck equation

J. Decker, Y. Peysson, et al. Phys. Plasmas 21 (2014) 092504

LHW absorption: Resonant and non-resonant absorption of the LH wave (C3PO/LUKE)



Deposited power for fragment i :

$$P_{abs}^{i}(\psi) = D_{\parallel i} \frac{\mathcal{P}_{i}}{\mathcal{P}_{i0}} \frac{c}{n_{\parallel i}} \left\langle \frac{\partial f}{\partial p_{\parallel}} \right|_{v_{\parallel} = c/n_{\parallel i}} \right\rangle$$

$$P_{abs} = \sum_{i} P^{i}_{abs}$$
 $P_{abs}(\psi) = \langle (\gamma - 1)mc^{2}Q_{LH}(f) \rangle$ $\gamma = \sqrt{1 + p^{2}/(mc)^{2}}$

$$\mathcal{P}_{i}^{new} = P_0 - \sum_{i'=1}^{i'=i} \left(\underbrace{P_{i'}^{NRCA} + P_{abs}^{i'}}_{\bullet} \right)$$

Iterations until $|\mathcal{P}_i - \mathcal{P}_i^{new}| / \mathcal{P}_i \leq 10^{-3}$ for each fragment of each ray : quasilinear self-consistency \rightarrow f and D_{II} are consistent.

If $\mathcal{P}_i \neq 0$ for the last fragment, the ray is too short and its length must be increased to get full power absorption if possible.

NRCA: non-resonant collisional absorption
 RLA: resonant Landau absorption



Resonant and non-resonant absorption of the LH wave: code validation (C3PO/LUKE)



WEST simulation : $\langle T_e \rangle$ = 0.41 keV, $\langle n_e \rangle$ = 5.7x10⁺¹⁹m⁻³



Resonant and non-resonant absorption of the LH wave: code validation





Comparison between LUKE simulations and fast elecron bremsstrahlung measurements (HXR)





2 LH antennas, multijunction



6 rows, 3.7 GHz, 9.2 MW

Tore Supra



E. Nilsson and J. Decker and Y. Peysson et al., Nucl. Fusion 53 (2013), 083018 Equipe TORE SUPRA, IAEA Conf. Proc. (1995) 105 Y. Peysson and J. Decker and E. Nilsson et al., PPCF 58 (2016) 044008 Peysson, Y, et al. J., Fus. Energy 39 (2020) 270

Y. Peysson et al.

Comparison between LUKE simulations and HXR measurements





1 LH antenna, full phasing



4 rows, 4.6 GHz, 2.5 MW

Liptac, J. et al., Rev. Sci. Instr., 77 (2006) 103504 I. H. Hutchinson et al. , Phys. Plasmas, 1 (1994) 1511



Y. Peysson and J. Decker and E. Nilsson et al., PPCF 58 (2016) 044008

Y. Peysson et al.

Comparison between LUKE simulations and HXR measurements



Unbridgeable spectral gap regimes by toroidal refraction : power spectrum should be already broad at the separatrix \rightarrow WEST, TRIAM-1M, HL-2A



Resonance condition : $V_{\parallel} = V_{\phi\parallel} = c/N_{\parallel}$

Peysson, Y, et al. J., Fus. Energy 39 (2020) 270

Y. Peysson et al.

Non-thermal bremsstrahlung during ECCD in presence of fluctuations



The reconstructed non-thermal bremsstrahlung count rate (central chord) is very close to the experimental HXR signal in the presence of fluctuations \rightarrow good match of CR versus chord number for $\sigma_f = 0.2$

The photon temperature is fairly independent of fluctuations

J. Decker, Y. Peysson, et al., EC-17 workshop (2012) Deurne, The Netherlands

Y. Peysson et al.

ICFRD, Varenna, Italy, 2021

CRPP

Towards multi-machines (-shots, -times) simulations

- So far, only "single" shots LUKE simulations have been performed → accurate calculations based on manually validated experimental data, but procedure is long and inappropriate for large multiparametric studies (*extraction of scaling laws, validate model robustness…*)
- Automatization of the whole chain of codes is mandatory for multi-machine, multi-shot or multi-time analysis (heterogeneous data)
- High modularity in the design when compatible with physics for an easy code maintenance and the possibility to introduce new physics or linking new codes (METIS → RAPTOR, ...)





 Each simulation requires large computing and data storage capabilities : calculations may last several hours, memory requirements may exceed several dozen of Megabytes per core and storage data size may reach several Gigabytes per simulation.



- A large number of simulations requires :
 - Distributed calculations capabilities with multiple core processors on local and remote machines
 - Fast symmetric ethernet connections (upload/download)





- The code must be launched by a single call at the top level for an easy symmetric integration : standalone run or integration in another codes
- A single structure of input parameters must be propagated in all SLUKE functions. It should be expressed in text form for easy exchange between users and track errors → control of each calculation everywhere
- Develop a basic object-oriented-like language → easy manipulation of all sets of input parameters.
- Transform any local function by a similar one with distributed remote capability with a simple syntax.
- No graphics except for specific debug : the structure of the main script must be consistent with the physics → adding new physics

Y. Peysson et al.





SLUKE timeline and input types







MatRemote MatLab toolbox for remote computing



- Enabling distributed and remote computing is one of the most important step towards automatic simulations → done for MatLab functions
- Embedded SSH (SCP) communication protocol + workload manager (PBS, SLURM, TORQUE, HTCONDOR,...)
- A dedicated toolbox has been designed for this purpose with a very simplified syntax :



The toolbox may be used for launching non-Matlab codes (Fortran, C, Python scripts, ...)



Remote computing set-up



Y. Peysson et al.

SLUKE : A single structure for all input parameters in a text script file

```
Structure of cells for
                                                   heterogeneous types of inputs
sparams.machine = {'WEST' 'TS' 'TCV'};
8
   _____
sparams.discharge.shot = {'55025' '32299' '11155025'};
sparams.discharge.tmin = {[3] [8] [9.5]};
sparams.discharge.tmax = {[3.1] [8.1] [9.9]};
                                                   Time slice or time intervals
sparams.discharge.nt = {[1] [1] [4]};
sparams.simul.id = {'Ohmic' 'LH flat-top' 'Collapse'};
sparams.simul.comment = {'' '' ''};
sparams.simul.enable = {[1] [1] [1]};
sparams.simul.enforce = {[0] [0] [0]};
                                                             Remote machine ID
sparams.simul.remote profile = {[17] [17] [5]};
sparams.simul.wait4results = {[0] [0] [0]};
sparams.simul.log = {[1] [0] [0]};
8
```





Toroidal MHD equilibrium

```
sparams.equil.id = {'METIS' 'METIS' 'METIS'};
sparams.equil.comment = {'metis calculation' 'metis calculation' 'metis calculation'};
sparams.equil.source = {'file' 'file' 'file'};
sparams.equil.code = {'''''};
sparams.equil.file =
{'55025_8_10_pradok_wok_ddnok_xlh023_dlh052_no_oxig_fne0_run17_new_tung_peak_LUKE.mat'
'55025_8_10_pradok_wok_ddnok_xlh023_dlh052_no_oxig_fne0_run17_new_tung_peak_LUKE.mat'
'55025_8_10_pradok_wok_ddnok_xlh023_dlh052_no_oxig_fne0_run17_new_tung_peak_LUKE.mat'
'55025_8_10_pradok_wok_ddnok_xlh023_dlh052_no_oxig_fne0_run17_new_tung_peak_LUKE.mat'
'sparams.equil.path = {'./INPUTS' './INPUTS' './INPUTS' './INPUTS' './INPUTS' './INPUTS' };
```

Ohmic electric field

```
sparams.ohm.id = {'METIS' 'METIS' 'METIS'};
sparams.ohm.comment = {'metis calculation' 'metis calculation' 'metis calculation'};
sparams.ohm.source = {'file' 'file' 'file'};
sparams.ohm.code = {'' '' ''};
sparams.ohm.file =
{'55025_8_10_pradok_wok_ddnok_xlh023_dlh052_no_oxig_fne0_run17_new_tung_peak_LUKE.mat'
'55025_8_10_pradok_wok_ddnok_xlh023_dlh052_no_oxig_fne0_run17_new_tung_peak_LUKE.mat'
'55025_8_10_pradok_wok_ddnok_xlh023_dlh052_no_oxig_fne0_run17_new_tung_peak_LUKE.mat'
'55025_8_10_pradok_wok_ddnok_xlh023_dlh052_no_oxig_fne0_run17_new_tung_peak_LUKE.mat'
'sparams.ohm.path = {'./INPUTS' './INPUTS' './INPUTS'};
```



A single structure for all input parameters







Easy structure manipulation for user-defined scripts



- sluke_params_preset : for preset sparams structures (examples, tests)
- sluke_params_value : get value of a field of the sparams structures
- sluke_params_script : generate a text script from a sparams structure
- sluke_params_time : expand time intervals in a sparams structure
- sluke_params_merge : group two sparams structures in a single one
- sluke_params_clone : clone an index of the sparams structures
- sluke_params_consistency : check the consistency of all fields of a sparams structure
- sluke_params_extract : extract a substructure in a sparams structure
- sluke_params_modify : modify fields in a sparams structure
- sluke_params_generator : user interactive creation of a sparams structure
- sluke_params_defaults : default sparams structures
- sluke_params_help : help of sparams structure

• ..



SLUKE main user script



```
%
% METIS/ALOHA/C3PO/LUKE/R5X2 simulation of WEST discharge #54802
%
clear all
close all
clc
%
make_sparams_WEST_54802;%load simulation parameters
%
sluke(sparams,mfilename);%main calculations
%
```

- May be put in a infinite loop to check simulations which is done and get back all results files. Or done manually. sparams is unchanged for a given set of simulations.
- Partial display may be done as far as simulations are progressively done in the same script. Data exchange by files only.
- Detailed results for a single shot may be displayed using LUKE display tool irunluke_jd.m









```
Simulation #4 [machine : WEST, shot : #54802, tmin : 5.7 (s), tmax : 5.8(s), ID : Collapse 2] ...
---> ALOHA simulation status (ID:WEST 54802_5.7_5.8_ALOHA_Q6A_ne_2) :
 - job #1 for WEST 54802 5.7 5.8 ALOHA Q6A ne 2 is completed.
 - job #2 for WEST 54802 5.7 5.8 ALOHA Q6A ne 2 is completed.
warning: min(zdP) < 0, correcting</pre>
---> is running.
Simulation #5 [machine : WEST, shot : #54802, tmin : 5.8 (s), tmax : 5.9(s), ID : Collapse 3] ...
---> ALOHA simulation status (ID:WEST 54802 5.8 5.9 ALOHA Q6A ne 2) :
 - job #1 for WEST 54802 5.8 5.9 ALOHA Q6A ne 2 is completed.
 - job #2 for WEST 54802 5.8 5.9 ALOHA Q6A ne 2 is completed.
warning: min(zdP) < 0, correcting
---> is running.
Simulation #6 [machine : WEST, shot : #54802, tmin : 5.9 (s), tmax : 6(s), ID : Collapse 4] ...
---> ALOHA simulation status (ID:WEST 54802 5.9 6 ALOHA Q6A ne 2) :
 - job #1 for WEST 54802 5.9 6 ALOHA Q6A ne 2 is completed.
 - job #2 for WEST 54802 5.9 6 ALOHA Q6A ne 2 is completed.
warning: min(zdP) < 0, correcting</pre>
---> is running.
                                                         Simulation after time expansion
   Y. Peysson et al.
                                           ICFRD, Varenna, Italy, 2021
                                                                                                #40
```



SLUKE status



- SLUKE is fully operational
- SLUKE is easy to use and fully customizable → based on MatLab text scripts
- Primarily designed for Tore Supra and WEST yet, but developments for other machines are scheduled.
- Open new capabilities for physics studies with quantitative assessments against experimental observations (if data are available)
 - Long time evolutions (RE dynamics, W collapses, ramp-up, synergies...)
 - Self-consistency between RF driven current with toroidal MHD equilibrium (resistive time)
 - Statistical studies using a large number of experimental results : *multi-time, multi-shot, multi-machine*



SLUKE example : WEST #55025



SLUKE simulations for 3 time intervals (Ohmic, LH flat-top, W collapse)



All equilibria are from METIS

J. F. Artaud et al., Nucl. Fusion, 58 (2018) 105001



Y. Peysson et al., Nucl. Fusion, 33 (1993) 1133

Y. Peysson et al.



Conclusions and prospects



- First principles modeling fast electron physics has reached a quite mature level with existing LUKE environment (ALOHA/METIS/C3PO/LUKE/R5X2)
- A new framework SLUKE has been developed for large scale quantitative first principles simulations : multi-time, multi-shot and multi-machine, thus allowing new physics studies.
- Further developments will concern LUKE kernel principally → LUKE 2 : finite banana width effects (*RF wave induced transport, self-consistent bootstrap current for non-Maxwellian distribution*,...) (theory is already done) and selfconsistent interactions between fast electrons and MHD modes (*principally for RE physics*)
- New synthetic diagnostics will be added to SLUKE framework.